

Dynamic polarization effects on the angular distributions of protons channeled through carbon nanotubes in dielectric media

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The best level of ordering and straightening of carbon nanotube arrays is often achieved when they are grown in a dielectric matrix, so such structures present the most suitable candidates for future channeling experiments with carbon nanotubes. Consequently, we investigate here how the dynamic polarization of carbon valence electrons in the presence of various surrounding dielectric media affects the angular distributions of protons channeled through (11, 9) single-wall carbon nanotubes. Proton speeds between 3 and 10 a.u., corresponding to energies of 0.223 and 2.49 MeV, are chosen with the nanotube's length varied between 0.1 and 1 μm . We describe the repulsive interaction between a proton and the nanotube's atoms in a continuum-potential approximation based on the Doyle-Turner potential, whereas the attractive image force on a proton is calculated using a two-dimensional hydrodynamic model for the dynamic response of the nanotube valence electrons, while assigning to the surrounding medium an appropriate (frequency dependent) dielectric function. The angular distributions of channeled protons are generated using a computer simulation method which solves the proton equations of motion in the transverse plane numerically. Our analysis shows that the presence of a dielectric medium can strongly affect both the appearance and positions of maxima in the angular distributions of channeled protons.

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I. INTRODUCTION

While progress in theoretical modeling and computer simulations of ion channeling through carbon nanotubes has reached a mature level, as recently reviewed in Ref. 1, efforts of experimentalists have only recently begun to bear fruit in this important research area. Because the best level of ordering and straightening of carbon nanotubes is achieved when they are grown in a dielectric matrix, such structures are perhaps the most suitable candidates for ion channeling through carbon nanotubes. It thus came as no surprise when Zhu *et al.* [2] recently reported the first experimental data on He^+ channeling through an array of well ordered, multi-wall carbon nanotubes (MWNTs) which were grown in a porous anodic aluminum oxide (Al_2O_3) membrane. On the other hand, carbon nanotubes have also been grown selectively within etched ion tracks in SiO_2 layers on Si by another experimental group [3], thus offering an interesting possibility for realization of ion channeling through individual, single-wall carbon nanotubes (SWNTs) at a wide range of ion energies. In addition, in many applications of carbon nanotubes it is desirable to have them embedded in a dielectric such as SiO_2 [4], or clamped by a metal shield [1] made of nickel, which is known to most readily bind to carbon nanotubes [5].

For ion channeling at the low (keV) and high (GeV) ends of the energy range, the surrounding material would predominantly serve as a passive container of carbon nanotubes when the dynamics of ion motion is concerned. However, ions moving with medium (MeV) energies will induce strong dynamic polarization of valence electrons in the nanotubes which in turn will give rise to a sizeable image force on the ions, as well as a considerable energy loss due to the collective, or plasma, electron excitations. The dynamic image force has been recently shown to give rise to the rainbow effect in the angular distributions of protons channeled through short (11, 9) single-wall [6] and double-wall carbon nanotubes [7] in free space, which is not otherwise observable in simulations of ion channeling through chiral carbon nanotubes using the continuum approximation for the interaction potential [1]. Obviously, the presence of dielectric media may affect these dynamic polarization forces, as well as the resulting ion trajectories, making the analysis of such effects in ion channeling through carbon nanotubes a timely task, which we take up in this contribution. In particular, we are interested here primarily in the effects of dielectric media on the dynamic image force on channeled ions and their angular distributions.

The rainbow effect occurs and plays an important role in photon scattering from water droplets [8, 9], nucleus-nucleus collisions [10, 11, 12], atom or ion collisions with atoms or molecules [13], electron-molecule collisions [14], atom or electron scattering from crystal surfaces [15, 16], and ion channeling in crystals [17, 18]. Moreover, the

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rainbow effect has been investigated recently in the context of grazing scattering of atoms from metal surfaces under channeling conditions by Schüller *et al.* [19] who showed that precise measurements of the well-defined maxima in the angular distributions of scattered atoms, attributed to the rainbow effect, can give detailed information on the interaction potential of the atoms with the metal surfaces. On the other hand, the theory of crystal rainbows has been formulated as the proper theory of ion channeling in thin crystals [20], and has been subsequently applied to ion channeling in short carbon nanotubes [21, 22, 23, 24]. It is therefore expected that, in analogy with the surface channeling experiments [19], measurements of the rainbow effect in carbon nanotubes may give precise information on both the atomic configuration and the interaction potentials within such structures, which are not completely known at present.

Previously reported simulations of ion channeling in carbon nanotubes [25, 26, 27] paid virtually no attention to the effects of dynamic polarization of the nanotube valence electrons. However, this process is expected to contribute to the ion energy loss and to give rise to strong image forces on the medium-energy ions [28], as was recently demonstrated in the computer simulations of angular distributions of protons channeled through chiral single-walled carbon nanotubes in vacuum [29]. The importance of the image force has also been emphasized in the related area of ion transmission through cylindrical channels in metals [30, 31, 32, 33, 34]. Whereas interesting parallels can be drawn between ion channeling through carbon nanotubes and ion transmission through capillaries, it is important to notice several crucial differences. Namely, while the lengths of capillaries in metals can be comparable to those of nanotubes considered here for ion channeling, their diameters are typically an order of magnitude, or more, larger than those of carbon nanotubes, making their aspect ratios considerably smaller. More importantly, the inner surfaces of such broad channels in metals usually appear to be quite rough, which does not seem to affect too much the transmission of slow, highly-charged ions through such structures [31, 32]. However, it is questionable whether conditions required for channeling of fast ions leading to the rainbow effect can be met in capillaries with such characteristics [19, 35]. On the other hand, in cases where carbon nanotubes are grown in amorphous channels in a dielectric such as Al_2O_3 [2] and SiO_2 [3], or are coated by an amorphous layer of metal [5, 36], it is precisely the regular atomic structure of carbon nanotube that acts as a smooth "sleeve", or "mantle" covering the underlying rough surface of the surrounding material, thus enabling ion channeling through such structures. It remains to be seen, however, whether large, multi-walled carbon nanotubes can be grown inside the broad capillaries in metals enabling some sort of ion channeling in their interior hollow regions.

We shall investigate here how dynamic polarization of carbon valence electrons influences the angular distribu-

tions of protons channeled in (11, 9) SWNTs with different dielectric media surrounding the nanotubes. We consider proton speeds between 3 and 10 a.u., and nanotube lengths between 0.1 and 1 μm . The image force acting on an ion moving in a nanotube surrounded by a dielectric medium has been recently calculated by means of a two dimensional (2D) hydrodynamic model for the carbon valence electrons, while the surrounding medium was described by a suitable frequency dependent dielectric function [37, 38]. In the present simulations, we shall use the van der Waals radius of a carbon atom (0.17 nm) to approximate the distance between the nanotube wall and various dielectric media [39, 40]. This value also agrees with our density functional theory (DFT) calculations of the average equilibrium separation between graphene and a Ni (111) surface, based on the methodology described in Ref. 41. Other details of our simulation are similar to those reported earlier [6, 7].

After outlining the basic theory used in modeling the dynamic polarization effects of carbon nanotubes, we shall discuss the results of our ion trajectory simulations and give our concluding remarks. Atomic units will be used throughout unless explicitly stated otherwise.

II. THEORY

The system under investigation is a proton moving through an (11, 9) SWNT surrounded by a dielectric medium. The z-axis coincides with the nanotube axis and the origin lies in its entrance plane. The initial proton velocity vector, \vec{v} , is taken to be parallel to the z-axis. Proton speeds between 3 and 10 a.u., corresponding to energies of 0.223 and 2.49 MeV, are considered, with the nanotube's length varied between 0.1 and 1 μm .

We also assume that the repulsive interaction between the proton and the nanotube atoms may be treated classically, using the Doyle-Turner expression for the proton-carbon atom interaction potential [42], averaged axially [43] and azimuthally [44]. The repulsive potential for proton channeling through the nanotube is then of the form

$$U_{\text{rep}}(r) = \frac{16\pi d Z_1 Z_2}{3\sqrt{3}l^2} \times \sum_{j=1}^4 a_j b_j^2 I_0(b_j^2 r d) \exp\{-b_j^2[r^2 + (d/2)^2]\}, \quad (1)$$

where $Z_1 = 1$ and $Z_2 = 6$ are the atomic numbers of proton and carbon atoms, respectively, $d = 2a$ is the nanotube diameter, l is the C-C bond length, r is the distance between the proton and nanotube axis, I_0 is the modified Bessel function, and $a_j = \{0.115, 0.188, 0.072, 0.020\}$ and $b_j = \{0.547, 0.989, 1.982, 5.656\}$ are fitting parameters in atomic units [42].

The dynamic polarization of the nanotube is treated by a 2D hydrodynamic model of the nanotube valence

electrons, based on a jellium-like description of the ion cores on the nanotube wall [28, 37]. This model includes both axial and azimuthal averaging consistent with our treatment of the repulsive interaction. The self energy, or the image potential, E_{self} , for a single ion of charge Z_1 at position $\vec{r}_0(t)$ is defined by

$$E_{\text{self}} = (Z_1/2)\Phi_{\text{ind}}(\vec{r}_0(t), t), \quad (2)$$

where $\Phi_{\text{ind}}(\vec{r}, t)$ is the potential at the point \vec{r} , given in cylindrical coordinates by $\vec{r} = \{r, \varphi, z\}$, which is induced in the system by the presence of ion. After performing the Fourier transform with respect to time, and following the method of Doerr and Yu [45], we consider the total electric potential to be the sum of the external perturbing potential, $\Phi_{\text{ext}}(\vec{r}, \omega)$, and the induced potential, $\Phi_{\text{ind}}(\vec{r}, \omega)$, due to polarization of the nanotube and the dielectric boundary by the proton, so that

$$\Phi(\vec{r}, \omega) = \Phi_{\text{ext}}(\vec{r}, \omega) + \Phi_{\text{ind}}(\vec{r}, \omega). \quad (3)$$

The Poisson equation then gives

$$\nabla^2 \Phi_{\text{ext}}(\vec{r}, \omega) = -4\pi\rho_{\text{ext}}(\vec{r}, \omega), \quad (4)$$

$$\nabla^2 \Phi_{\text{ind}}(\vec{r}, \omega) = 4\pi[n_1(\vec{r}_a, \omega)\delta(r-a) - \sigma_b(\vec{r}_b, \omega)\delta(r-b)], \quad (5)$$

where \vec{r}_a is a position on the nanotube of radius a given by $\vec{r}_a = \{a, \varphi, z\}$, \vec{r}_b is a position on the boundary of the dielectric of radius b given by $\vec{r}_b = \{b, \varphi, z\}$, $n_1(\vec{r}_a, \omega)$ is the induced electron number density (per unit area) on the nanotube, and $\sigma_b(\vec{r}_b, \omega)$ is the polarization charge density (per unit area) induced on the boundary of the dielectric.

We may denote the Fourier transform in cylindrical coordinates of an arbitrary function $A(r, \varphi, z, \omega)$ by

$$A(r, \varphi, z, \omega) = \sum_{\mathbf{m}} \int \frac{dk}{(2\pi)^2} e^{im\varphi} e^{ikz} \tilde{A}(r, m, k, \omega). \quad (6)$$

The Green's function in cylindrical coordinates is then

$$\frac{1}{\|\vec{r} - \vec{r}'\|} = \sum_{\mathbf{m}} \int \frac{dk}{(2\pi)^2} e^{im(\varphi - \varphi')} e^{ik(z - z')} g(r, r', m, k), \quad (7)$$

where $g(r, r', m, k)$ is the radial Green's function,

$$g(r, r', m, k) = 4\pi I_m(kr_{<}) K_m(kr_{>}),$$

with $r_{<} = \min\{r, r'\}$, $r_{>} = \max\{r, r'\}$, and I_m and K_m being the modified Bessel's functions of the first and second kind, respectively.

The Fourier transform of the external perturbing potential due to a single proton of charge $Z_1 = 1$ moving parallel to the nanotube axis with constant speed v , such that $\vec{r}_0(t) = \{r_0, \varphi_0, vt\}$, is given by

$$\tilde{\Phi}_{\text{ext}}(r) = \frac{2\pi Z_1}{\varepsilon_{\text{nt}}} g(r, r_0, m, k) \delta(\omega - kv) e^{-im\varphi_0}, \quad (8)$$

where ε_{nt} is the background optical dielectric constant for the nanotube (for which we use $\varepsilon_{\text{nt}} = 1$), m, k and ω are the angular oscillation mode, longitudinal wave number and angular frequency of an elementary excitation of the nanotube atoms valence electrons treated as an electron gas. Note that one may set $\varphi_0 = 0$ because of the axial symmetry of our model for nanotube. The Fourier transform of the induced potential is given by [37]

$$\tilde{\Phi}_{\text{ind}}(r) = \frac{-a\tilde{n}_1}{\varepsilon_{\text{nt}}} [g(r, a, m, k) + b\Re g(r, b, m, k)g'(b, a, m, k)] + b\Re g(r, b, m, k) \frac{\partial \tilde{\Phi}_{\text{ext}}}{\partial r}|_b, \quad (9)$$

where $g'(r, r', m, k) \equiv \frac{\partial}{\partial r} g(r, r', m, k)$, and the Fourier transform of the induced electron number density on the nanotube is

$$\tilde{n}_1 = \frac{\tilde{\Phi}_{\text{ext}}(a) + bg(a, b, m, k)\Re \frac{\partial \tilde{\Phi}_{\text{ext}}}{\partial r}|_b}{\chi^{-1} + \frac{a}{\varepsilon_{\text{nt}}} [g(a, a, m, k) + b\Re g(b, a, m, k)g'(b, a, m, k)]}. \quad (10)$$

Here we have defined the response function of the polarization charge due to the external electric field in the radial direction on the outer boundary of the medium, with dielectric function ε_ω , by

$$\Re \equiv \frac{\varepsilon_\omega - \varepsilon_{\text{nt}}}{4\pi[\varepsilon_{\text{nt}} + (\varepsilon_{\text{nt}} - \varepsilon_\omega)kbI_m(kb)K'_m(kb)]}. \quad (11)$$

The response function, χ , for the induced electron density on the nanotube due to the total electric potential, defined by $\tilde{n}_1 = \chi\tilde{\Phi}$, is given in the 2D hydrodynamic model by

$$\chi \equiv \frac{n_0(k^2 + m^2/a^2)}{\alpha(k^2 + m^2/a^2) + \beta(k^2 + m^2/a^2)^2 - \omega(\omega + i\gamma)}, \quad (12)$$

where n_0 is the equilibrium number density of all four carbon valence electrons ($n_0 \approx 0.428$ a.u.), $\alpha = \pi n_0$, $\beta = 1/4$, and we take the limit $\gamma \rightarrow 0^+$ [37].

We note that the above theory yields the self energy (image potential), $E_{\text{self}}(r_0)$, as a stationary function in the proton's moving frame of reference, which only depends on proton's radial position r_0 within an infinitely long nanotube. In that respect, it should be possible to limit our considerations to nanotubes which are long

enough so that we may ignore the edge effects on the image potential at the entrance and exit planes and, at the same time, short enough that the total energy losses of channeled protons may be neglected. Therefore, when calculating the dynamic image force on a proton one may safely consider its longitudinal velocity component as constant equal to its initial speed v , while changes in the perpendicular components of the proton velocity \vec{u} can be neglected under channeling conditions. Consequently, one may consider the radial position \vec{r} of a channeled proton to evolve adiabatically under the action of an axially symmetric force field, $F(r) = F_{\text{rep}}(r) + F_{\text{image}}(r)$, where $F_{\text{rep}}(r) = -dU_{\text{rep}}(r)/dr$ and $F_{\text{image}}(r) = -dE_{\text{self}}(r)/dr$. Because our numerical calculations of proton trajectories will be executed under the assumption of a homogeneous, mono-directional beam of protons incident in the direction parallel to the nanotube axis, the resulting simulation code will be essentially two-dimensional (2D). The effects on proton channeling coming from a divergent beam and non-parallel incidence will be studied by a full 3D code in future reports.

It should be also mentioned that the assumption that proton charge remains fixed at $Z_1 = 1$, which is used in our channeling simulations, needs careful consideration. Making analogy with the analysis of experiments on grazing scattering of protons on an Al surface [46] and referring to the data on proton transmission through carbon foils [47], one may expect that the $Z_1 = 1$ charge state would be the most dominant fraction for protons channeled in carbon nanotubes at the speeds in excess of $v = 3$. Nevertheless, simultaneous measurements of the angular distributions of transmitted particles in different charge states could reveal a wealth of information on both the image interactions and the charge transfer processes taking place in short nanotubes, in close analogy with the experiments done by Winter [35, 46]. On the other hand, for ion channeling through longer nanotubes, the image force itself can be quite strongly affected by the dynamics of the charge-changing events near the nanotube wall, as was shown recently for grazing scattering of protons from an Al surface [48]. The effects of charge transfer will be included in our future ion channeling simulations.

The angular distributions of transmitted protons are generated using a Monte-Carlo computer simulation method. The Cartesian components of the proton impact parameter, x_0 and y_0 , are chosen from a random uniform distribution within the nanotube cross-sectional area. With the bond length between the nanotube atoms being 0.144 nm [49], we obtain for the radius of the (11, 9) nanotube of $a = 0.689$ nm. Any protons with an impact point inside the annulus with radii in the interval $[a - a_{\text{sc}}, a]$, where $a_{\text{sc}} = [9\pi^2/(128 Z_2)]^{1/3} a_0$ is the screening length (with a_0 being Bohr's radius), are treated as if they were backscattered and are disregarded from the simulation. The initial number of protons used is 3 141 929.

The Cartesian components of the proton scattering angle, i.e., of the deflection function, Θ_x and Θ_y , are ob-

tained via the expressions $\Theta_x = u_x/v$ and $\Theta_y = u_y/v$, where u_x and u_y are the Cartesian components of the final perpendicular velocity vector, \vec{u} , obtained in our simulation of transmitted protons. It has been demonstrated that the proton channeling in nanotubes can be analyzed successfully via the corresponding mapping of the impact parameter plane, the x_0y_0 plane, to the scattering angle plane, the $\Theta_x\Theta_y$ plane. However, as the total interaction potential in the case under consideration is axially symmetric and the incident protons are moving parallel to the nanotube axis, the analysis of the mapping may be reduced to the analysis of the scattering angle, $\Theta = (\Theta_x^2 + \Theta_y^2)^{1/2}$, as a function of the impact parameter, $r_0 = (x_0^2 + y_0^2)^{1/2}$. Therefore, we may take $y_0 = 0$, and analyze the deflection function $\Theta_x(x_0)$ only. The extrema of this function are the rainbow extrema, and the corresponding singularities appearing in the angular distribution of channeled protons are the rainbow singularities [6].

III. RESULTS AND DISCUSSION

In this section we shall first discuss in Figures 1 and 2 respectively the image force and the total interaction force for a proton channeled in an (11, 9) SWNT in vacuum and encapsulated by SiO_2 , Al_2O_3 and Ni channels. Subsequently, we shall analyze the dynamic polarization effects on the angular distributions of protons after channeling at a speed of $v = 5$ a.u. through an (11, 9) nanotube placed in vacuum and in SiO_2 for three nanotube lengths, $L = 0.1, 0.3$, and $0.5 \mu\text{m}$ in Figures 3, 4 and 5, respectively. This analysis will be followed by a comparison of the dynamic polarization effects for different proton speeds but with a fixed dwell time, $T = L/v = 0.1 \mu\text{m}/v_{\text{B}} = 0.04571$ ps (with v_{B} being the Bohr speed), for nanotubes in vacuum and in SiO_2 . Next, we shall compare the effects of different media, namely SiO_2 , Al_2O_3 , and Ni, for the case of $L = 0.8 \mu\text{m}$, $v = 8$ a.u., as shown in Figures 6, 7 and 8, respectively. Finally, we shall comment on the zero degree focusing (ZDF) effect for proton speeds $v = 3$ a.u., $v = 5$ a.u. and $v = 8$ a.u. for nanotubes of various lengths, placed in vacuum and in SiO_2 , as shown in Figure 9. Qualitative analysis of the results will also be presented in terms of typical proton trajectories in the nanotube in vacuum and in SiO_2 , shown in Figures 10 and 11.

Figure 1 gives the image force of a proton traveling paraxially at $r = 3$ (lower), 7 (middle) and 10 a.u. (upper), with speed v , due to an (11, 9) SWNT in vacuum (dashed curves) and encapsulated by three dielectric materials (solid curves). The radius of this nanotube is $a \approx 13.01$ a.u. while the radius of the dielectric channel is $b \approx a + 3.21$ a.u. ≈ 16.22 a.u., where we have used carbon's van der Waals radius (≈ 3.21 a.u.) to approximate the separation between the nanotube and the nearby dielectric surface. In the case a nickel channel surrounding the nanotube, DFT based structural minimization cal-

culations performed using SIESTA [41] for graphene on a Ni(111) surface also yielded a separation of approximately 0.17 nm. In Fig. 1(a) we describe the surrounding silicon dioxide (SiO_2) by a dielectric constant of 3.9 [50], in Fig. 1(b) we model the dielectric response of anodic aluminum oxide (Al_2O_3) following the method described in Ref. 30, and in Fig. 1(c) we model the dielectric response of Ni metal following the method described in Ref. 51. The solid and dashed curves in Figs. 1 indicate that, for proton speeds below $v \approx 3$ a.u., the dielectrics have little influence on the image force, for proton speeds between $v \approx 3$ a.u. and $v \approx 6$ a.u. the image force is somewhat smaller in the presence of dielectrics, while, for speeds above $v \approx 6$ a.u. the image force is increased compared to the vacuum case. These results may be explained by the plasmon hybridization in the nanotube-dielectric system, as previously described in Ref. 37. In brief, protons moving at speeds below $v \approx 3$ a.u. do not induce plasma oscillations in the nanotube, so that the dielectric media are completely screened from the ion and do not influence the ion's self energy. Above this speed plasma oscillations appear, giving incomplete screening of the dielectric media by the nanotube via strong plasmon hybridization. As a result, dielectric media strongly affect the proton's self energy and the resulting image force at intermediate proton speeds. At high speeds, the nanotube becomes increasingly transparent to the proton, so that the dynamic-polarization effects tend to be dominated by the surrounding dielectric media. This is further elaborated in Fig. 1(c), where we also show the image force on proton at the same three distances inside Ni channels containing *no* encapsulated nanotube. Specifically, we display the results for a channel of radius $b = 16.22$ a.u. (dotted lines) showing how dynamic polarization of nickel becomes prominent in the combined nanotube-channel system only at high speeds. For the sake of comparing different channeling systems, we also show in Fig. 1(c) the results for image force in a Ni channel with its radius equal to that of a (11, 9) nanotube, $b = a = 13.01$ a.u. (thin solid lines). One can see that the image forces inside the nanotube in vacuum and in a Ni channel of the same radius have generally comparable magnitudes, with the case of a Ni channel undergoing stronger polarization at high proton speeds, say $v > 6$ a.u., and the nanotube providing a stronger image force at the intermediate to low proton speeds, say $v \propto 2$ -5 a.u.

We further analyze in Fig. 2 the total force on proton channeling, $F = F_{\text{rep}} + F_{\text{image}}$ as a function of the position x (in a.u.) across the nanotube radius, for proton speeds of (a) $v = 3$ a.u., (b) $v = 5$ a.u., and (c) $v = 8$ a.u. Here, the dashed curves denote the case of an (11, 9) nanotube in vacuum, while the solid curves of various thicknesses denote the effects of the three surrounding media, SiO_2 , Al_2O_3 and Ni, by thin, medium, and thick solid curves, respectively. The lower branches of these curves show the behavior of the image force F_{image} alone close to the nanotube, while the upper branches show

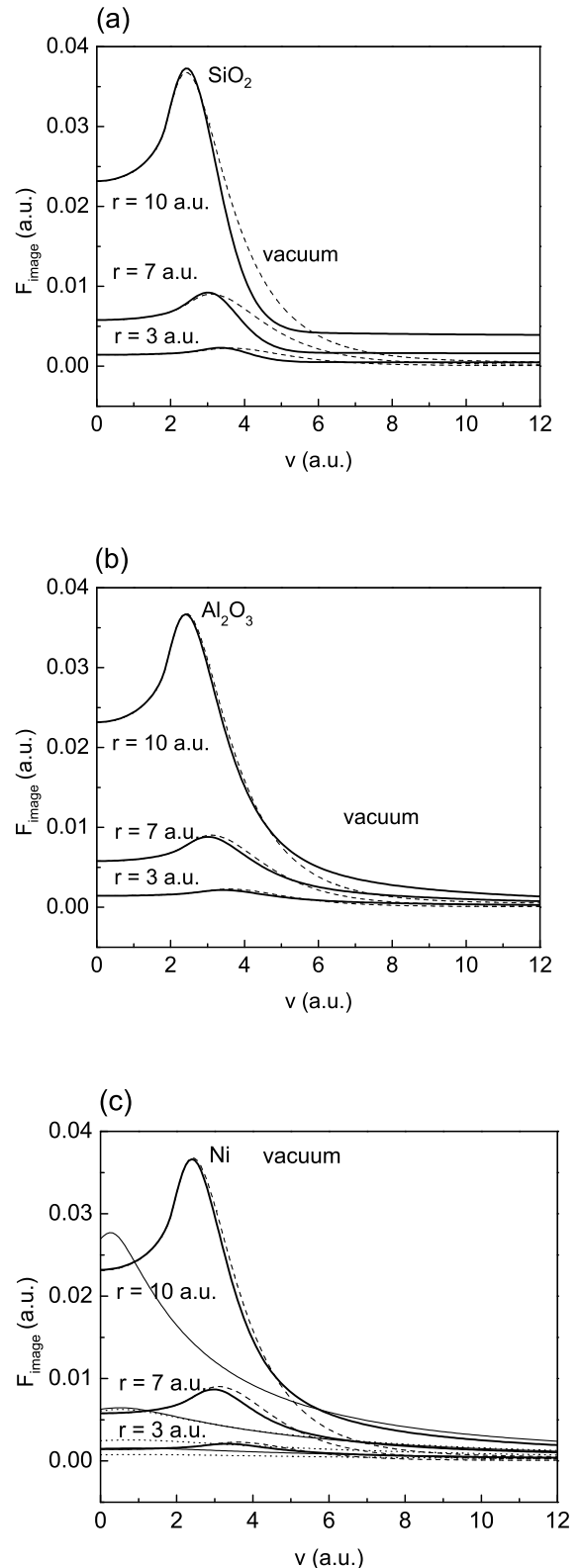


FIG. 1: The image force of a proton traveling paraxially at three distances from the nanotube axis: $r = 3$ (lower), 7 (middle) and 10 a.u. (upper), as a function of proton speed v in a.u., due to an (11, 9) SWNT in vacuum (dashed curves) and encapsulated by an (a) SiO_2 channel, (b) Al_2O_3 channel and (c) Ni channel (solid curves). The radius of the nanotube is $a = 13.01$ a.u. and the radius of the dielectric channel is $b = 16.22$ a.u. In panel (c) we also show the image force for the same three distances inside Ni channels without encapsulated nanotube for two channel radii: $b = 13.01$ a.u. (thin solid

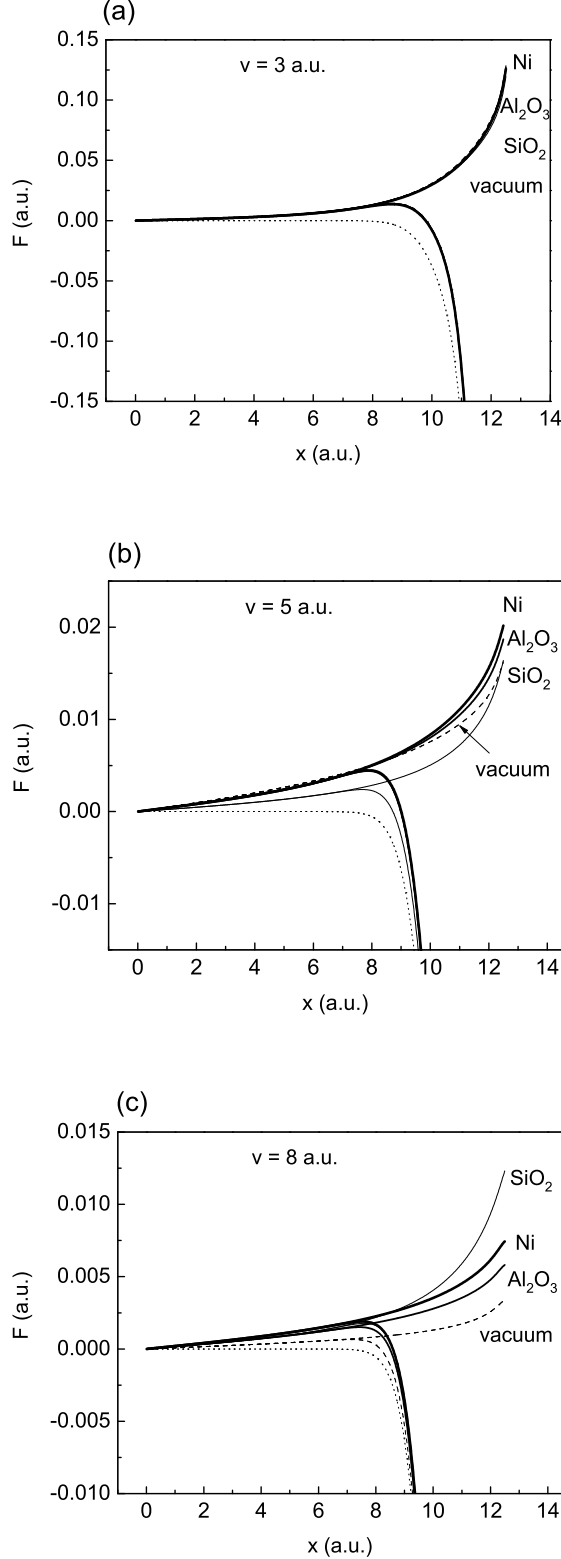


FIG. 2: The image force of a proton channeled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by SiO_2 , Al_2O_3 and Ni channels (thin, medium, and thick solid curves) as functions of the proton position x in a.u. across the nanotube radius, for three proton speeds: (a) $v = 3$ a.u., (b) $v = 5$ a.u. and (c) $v = 8$ a.u. The dotted curve gives the repulsive force, F_{rep} , while the lower branches of solid and dashed curves give the attractive image force alone, F_{image} , and the upper branches give the total force F , due to an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by the three channels (solid curves). The radius of the nanotube is $a = 13.01$

the total force F as a result of adding the bare repulsive force F_{rep} (shown by dotted lines) to the image force. Although close to the nanotube the total force is obviously dominated by the repulsive force due to the carbon atoms, the effects of the dielectric media on the attractive interactions due to the image force are greatly affected by both the proton speed and the type of the surrounding material. Figure 2(a) shows practically no effects of the dielectric media for a proton speed of $v = 3$ a.u., as expected from Fig. 1. At an intermediate proton speed of $v = 5$ a.u., while the curves in Fig. 2(b) for Al_2O_3 , Ni and vacuum are very close to each other, especially in the inner part of the nanotube, the case of SiO_2 displays a surprisingly weaker image force almost up to the nanotube wall. On the other hand, for $v = 8$ a.u., the image forces shown in Fig. 2(c) have similar values for all three dielectric media, especially in the inner part of the nanotube, whereas the image force for the case of nanotube in vacuum is substantially weaker at all distances. As commented in reference to Fig. 1, the nanotube becomes increasingly transparent at high proton speeds, so that any dynamic-polarization effects will be due to the polarization of the surrounding dielectrics [37]. This implies that, while the image interaction will be heavily suppressed at high proton speeds for the nanotube in vacuum, it can remain operational in the presence of surrounding media and, in fact, will be dominated by their dielectric properties as if carbon nanotube was not there. Thus, since the image force is crucial for the appearance of rainbows and the ZDF in ion angular distributions after channeling through short carbon nanotubes, we expect strong effects of the surrounding media, especially at higher (but still non-relativistic) speeds.

In Figures 3-5, we show the results of proton channeling through the nanotube in vacuum (dashed curves) and encapsulated by a SiO_2 channel (solid curves), by both the deflection function $\Theta_x(x_0)$ in panels (a), and the corresponding angular distributions in panels (b). In Fig. 3, where the proton speed is $v = 5$ a.u. and the nanotube length is $L = 0.1 \mu\text{m}$, we find a pair of very shallow extrema, labeled 1, of the dashed curve in panel (a), whereas the solid curve does not exhibit such extrema. As a consequence, the corresponding angular distributions in Fig. 3(b) display, besides massive central peaks, also two very small rainbow peaks, also labeled 1, in the case when the nanotube is in vacuum (dashed curve). However, we find no rainbow peaks when the nanotube is surrounded by SiO_2 (solid curve). On the other hand, the yield in the central maximum for the SiO_2 case is found to be almost three times larger than in the case of a nanotube in vacuum. These findings can be explained by examining the results in Fig. 2(b) shown by the thin solid curve for the SiO_2 case in comparison to those shown by the dashed curve for a nanotube in vacuum. The rainbow effect is missing in the case of SiO_2 because the image force is too weak compared to the vacuum case, and the protons are not pulled far enough from their initial direction in such a short nanotube. On the

other hand, the image potential well (not shown here) is found to be shallower and broader in the case of SiO_2 implying that a larger fraction of the incident protons will be very near the initial direction, giving more flux of undeflected particles than in the vacuum case. Increasing the nanotube length to $L = 0.3 \mu\text{m}$, as shown in Fig. 4, amounts to a shift of the extrema 1 in the vacuum case (dashed curves), and also to the appearance of a pair of extrema, labeled by 1_d , in the solid curves due to the image force when the nanotube is in a dielectric medium (SiO_2). A further increase of the nanotube length to $L = 0.5 \mu\text{m}$, as shown in Fig. 5, gives rise to multiple rainbows when the carbon nanotube is in vacuum. As discussed in Ref. 6, the rainbows labeled by 1 belong to the first class (rainbow trajectories which have experienced one deflection within the image-generated potential well), while the rainbows labeled by $2'$ and $2''$ belong to the second class (rainbow trajectories which have experienced two deflections within the potential well). However, no new rainbow peaks appear in the solid curves shown in Fig. 5 when the nanotube is in SiO_2 , besides the pair of peaks labeled by 1_d , which are now shifted in comparison to those in Fig. 4. This inability of the image force to create multiple rainbows in the case of the surrounding SiO_2 channel can again be explained by comparing the thin solid line for SiO_2 with the dashed line for a nanotube in vacuum, shown in Fig. 2(b).

We further concentrate on the velocity dependencies in the effects of dielectrics on the image force, while eliminating the cumulative effects on ion deflection due to the increasing nanotube length. This is done by looking into various cases with fixed dwell time, $T = L/v = 0.1 \mu\text{m}/v_B$, for nanotubes in vacuum and in SiO_2 . Considering low proton speeds, say below $v \approx 3 \text{ a.u.}$, we note that the results for all three surrounding media (SiO_2 , Al_2O_3 , or Ni) should be virtually identical to the results for an (11, 9) nanotube in vacuum. This is because protons at such speeds do not induce plasma oscillations in the carbon nanotube, so that the influence of the dielectric media is completely screened, as shown in Figs. 1 and 2(a). The results for the combination of parameters $L = 0.3 \mu\text{m}$, $v = 3 \text{ a.u.}$ are displayed in Figure 4 of Ref. 6, where one can see five pairs of the extremal points, labeled by 1, $2'$, $2''$, $3'$ and $3''$, which result from one (1), two ($2'$ and $2''$) and three ($3'$ and $3''$) deflections of the rainbow trajectories within the image-generated potential well. For the combination of parameters $L = 0.5 \mu\text{m}$, $v = 5 \text{ a.u.}$, as shown in Fig. 5, one notices a significant depletion of the number of rainbow peaks, down to three pairs (1, $2'$ and $2''$) for the nanotube in vacuum, and only one pair (1_d) for surrounding SiO_2 . The further reduction of the number of rainbow peaks with increasing proton speed is illustrated in Fig. 6 for the combination of parameters $L = 0.8 \mu\text{m}$, $v = 8 \text{ a.u.}$ Here, we notice that the massive central peak is wider than in Fig. 5, while the rainbow effect has completely disappeared for the nanotube in vacuum. This is due to the diminished

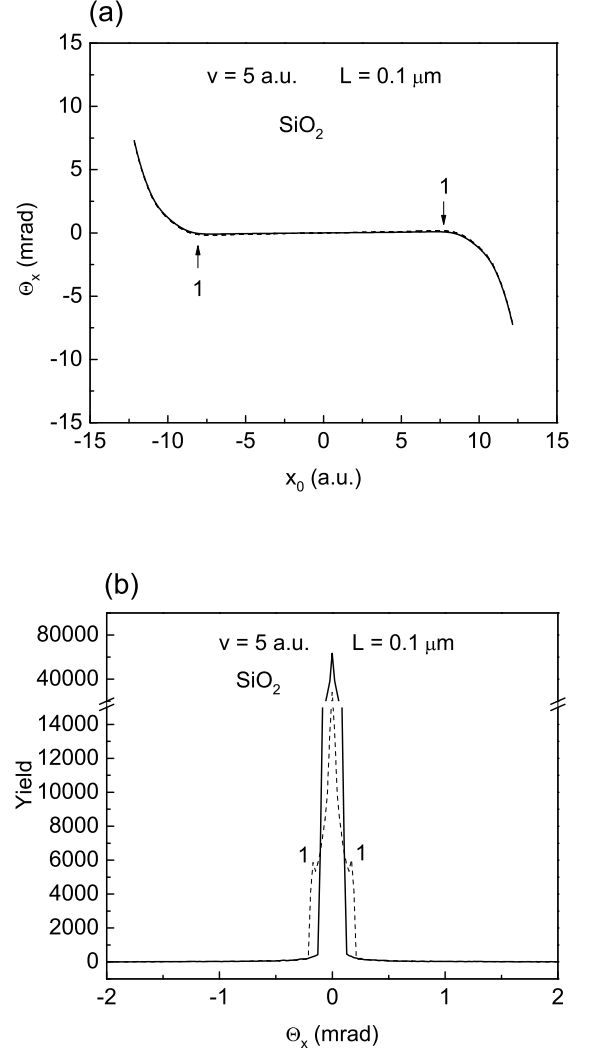


FIG. 3: The (a) deflection functions and (b) corresponding angular distributions of protons channeled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by a SiO_2 channel (solid curve). The proton speed is $v = 5 \text{ a.u.}$, the nanotube length is $L = 0.1 \mu\text{m}$, the nanotube radius is $a = 13.01 \text{ a.u.}$, and the dielectric channel radius is $b = 16.22 \text{ a.u.}$ The angular distribution's bin size is 0.0213 mrad .

image force on protons at such a high speed. On the other hand, the one rainbow peak (1_d) from Fig. 5 has remained in Fig. 6 for the case of a nanotube surrounded by SiO_2 , although this peak is now very small. This persistence of the rainbow peak for a surrounding dielectric can be explained by the "transparency" of nanotubes at high proton speeds [37], where the image force is dominated by the polarization of the surrounding dielectric, as shown in Fig. 2(c).

We also compare the case of proton speed $v = 8 \text{ a.u.}$ and nanotube length $L = 0.8 \mu\text{m}$ for the nanotube in SiO_2 , Al_2O_3 and Ni , as shown in Figures 6, 7 and 8,

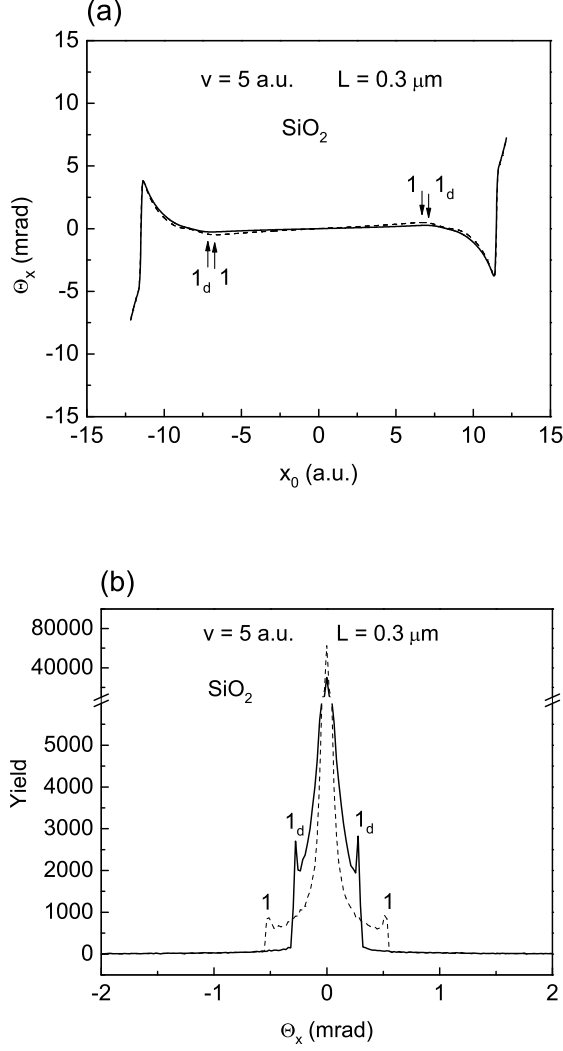


FIG. 4: The (a) deflection functions and (b) corresponding angular distributions of protons channeled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by a SiO_2 channel (solid curve). The proton speed is $v = 5$ a.u., the nanotube length is $L = 0.3 \mu\text{m}$, the nanotube radius is $a = 13.01$ a.u., and the dielectric channel radius is $b = 16.22$ a.u. The angular distribution's bin size is 0.0213 mrad.

respectively. One notices that the positions of the rainbow extrema, labeled by 1_d , hardly change for the solid curves shown in Figs. 6-8 for different dielectrics. This can be explained by the relatively close proximity of the three image-force curves for nanotubes in dielectrics, shown in Fig. 2(c) for all three dielectrics, at distances where extremal points occur in the corresponding deflection curves, as shown in Figs. 6-8.

As evidenced in Figs. 3-8, the effects of dielectric media on the dynamic polarization of carbon nanotubes also affect quite strongly the central peaks in the angular distributions of channeled ions. We therefore analyze next

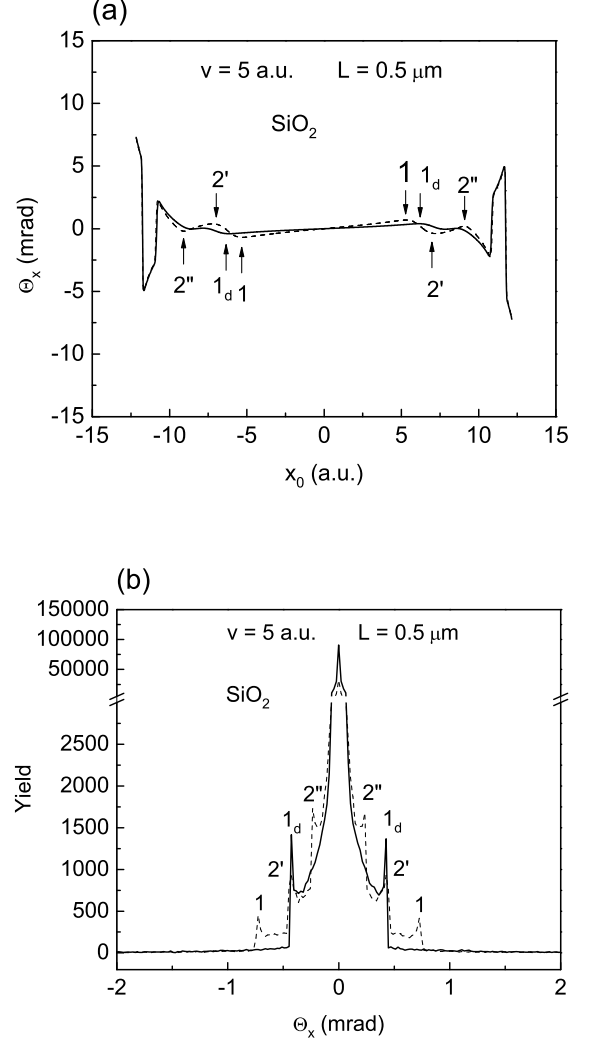


FIG. 5: The (a) deflection functions and (b) corresponding angular distributions of protons channeled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by a SiO_2 channel (solid curve). The proton speed is $v = 5$ a.u., the nanotube length is $L = 0.5 \mu\text{m}$, the nanotube radius is $a = 13.01$ a.u. and the dielectric channel radius is $b = 16.22$ a.u. The angular distribution's bin size is 0.0213 mrad.

how these effects change the ZDF in the case an (11, 9) nanotube in vacuum and in a SiO_2 channel. We first note that our simulations of proton channeling through carbon nanotubes without the image force, when proton trajectories are governed only by the repulsive Doyle-Turner potential, did not yield any periodic peaking of ion directions parallel to the nanotube. This is explained by the short range of the Doyle-Turner potential, which is very steep near the nanotube walls, so that protons with different impact parameters undergo transversal oscillations with a wide range of periods. Therefore, there is no single frequency of such oscillations that may give rise to the pe-

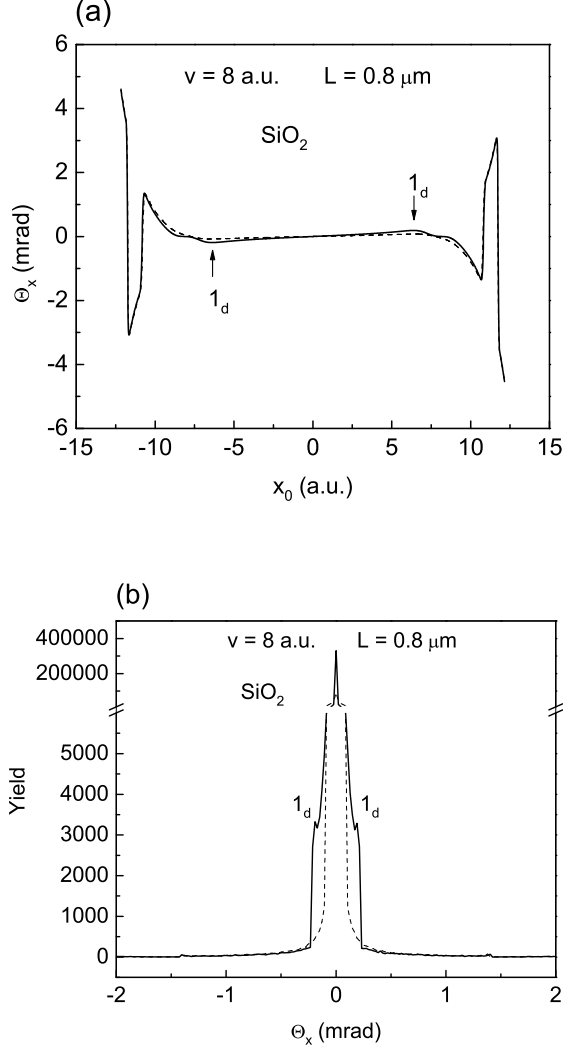


FIG. 6: The (a) deflection functions and (b) corresponding angular distributions of protons channelled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by a SiO_2 channel (solid curve). The proton speed is $v = 8$ a.u., the nanotube length is $L = 0.8 \mu\text{m}$, the nanotube radius is $a = 13.01$ a.u. and the dielectric channel radius is $b = 16.22$ a.u. The angular distribution's bin size is 0.0213 mrad.

riodic peaking of ion directions parallel to the nanotube when their length increases. When the image potential is included in our simulations, one finds parabolic regions in the total potential near the minima. This allows for a broader range of proton impact parameters that would give oscillations in the transversal directions at almost the same frequency. When the trajectories of such protons become almost parallel to the entrance beam, one finds the effect of ZDF. In our simulations, we use as a criterion for the ZDF that the proton speeds in the transverse directions are $v_t < 10^{-5}$ a.u.

Figure 9 illustrates the effects of a surrounding medium

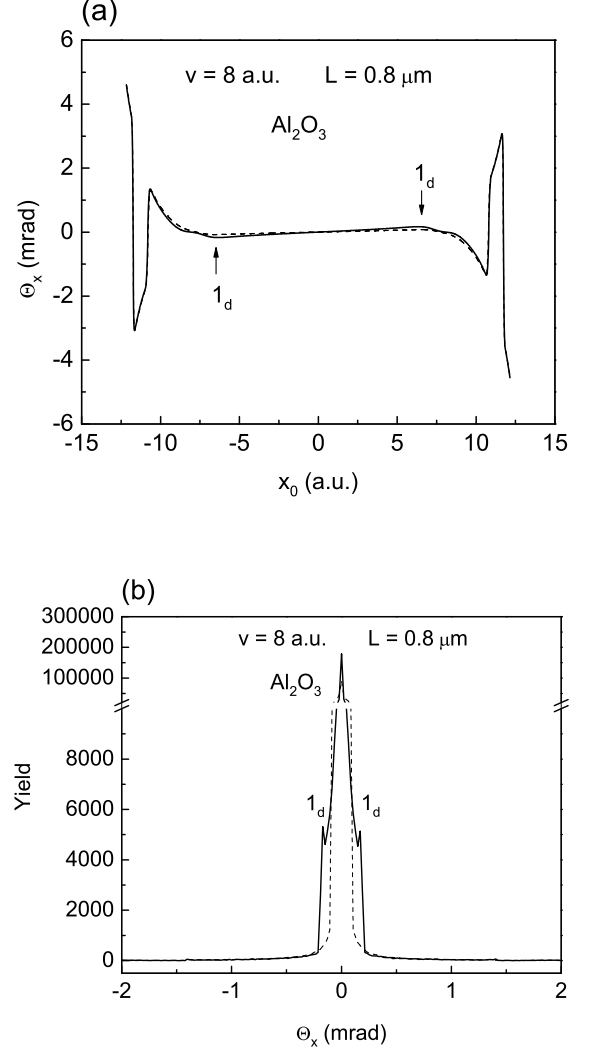


FIG. 7: The (a) deflection functions and (b) corresponding angular distributions of protons channelled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by an Al_2O_3 channel (solid curve). The proton speed is $v = 8$ a.u., the nanotube length is $L = 0.8 \mu\text{m}$, the nanotube radius is $a = 13.01$ a.u. and the dielectric channel radius is $b = 16.22$ a.u. The angular distribution's bin size is 0.0213 mrad.

on the ZDF by showing the dependence of proton yield (for $v_t < 10^{-5}$ a.u.) on the dwell time, L/v , for protons channelled in an (11, 9) SWNT in vacuum and encapsulated by a SiO_2 channel, where the proton speeds are (a) $v = 3$ a.u., (b) $v = 5$ a.u. and (c) $v = 8$ a.u. While the surrounding dielectric does not effect the ZDF for a proton speed of $v = 3$ a.u., we notice strong effects on the ZDF for proton speeds $v = 5$ a.u. and $v = 8$ a.u. when compared to the case of the nanotube in vacuum. Specifically, the period of the ZDF occurrence is seen to increase steadily with increasing proton speed in the latter case, owing to the weakening image interaction with

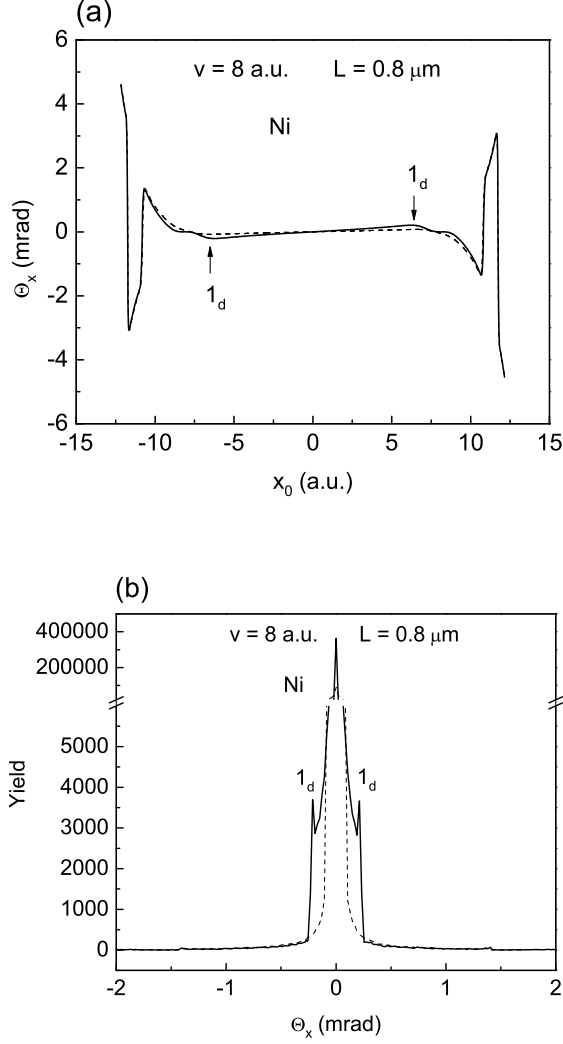


FIG. 8: The (a) deflection functions and (b) corresponding angular distributions of protons channelled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by a Ni channel (solid curve). The proton speed is $v = 8$ a.u., the nanotube length is $L = 0.8 \mu\text{m}$, the nanotube radius is $a = 13.01$ a.u. and the dielectric channel radius is $b = 16.22$ a.u. The angular distribution's bin size is 0.0213 mrad.

the nanotubes in vacuum, whereas this increase seems to saturate at higher proton speeds for nanotubes in a SiO_2 channel. Realizing that the ZDF peaks appear more frequently when the image force is stronger, one can easily refer to Figs. 2 (b) and (c) to explain why the first ZDF peaks for the nanotubes in SiO_2 appear in Figs. 9 (b) and (c), respectively, after and before the first peaks for the nanotubes in vacuum.

As regards the yields in the central maxima on the (b) panels of Figs. 4-6, we have seen for the case of $v = 5$ a.u. and $L = 0.3 \mu\text{m}$, shown in Fig. 4(b), that the yield when the nanotube is in vacuum is about twice the

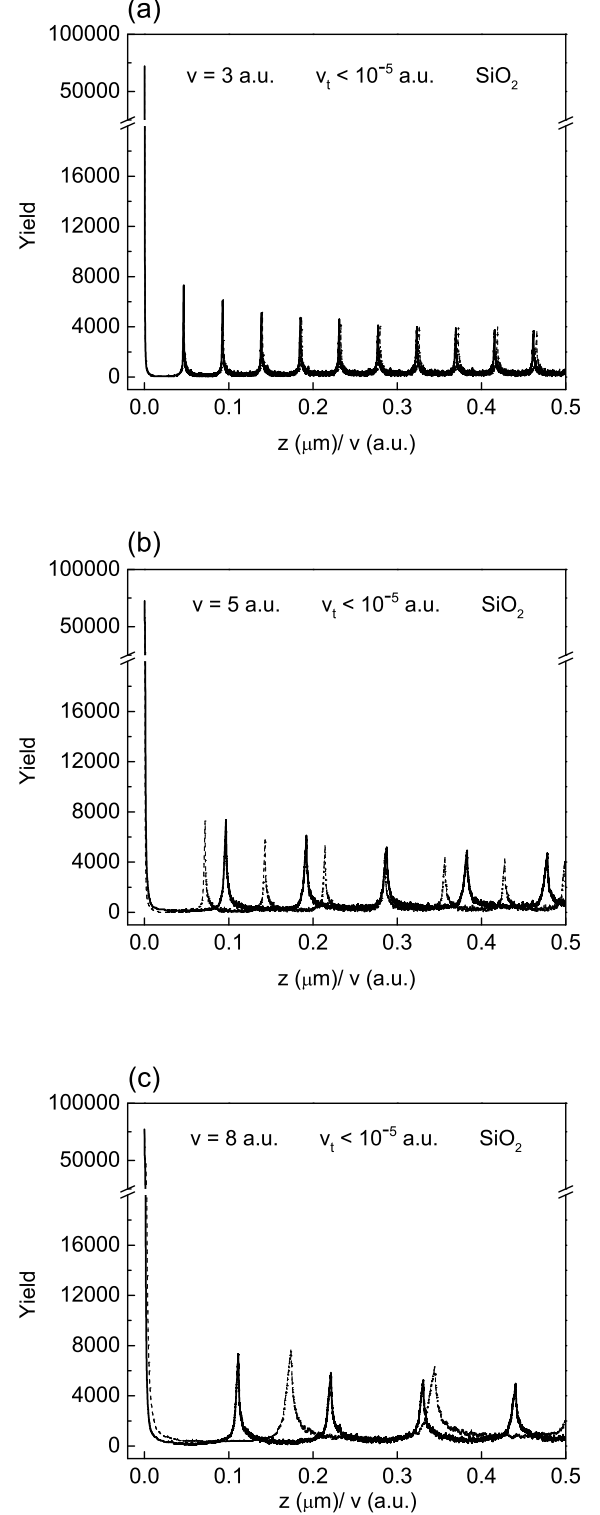


FIG. 9: Dependence of the zero-degree focusing (ZDF) versus dwell time L/v (in units of $\mu\text{m}/v_b = 0.4571$ ps) for protons channelled in an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by a SiO_2 channel (solid curve). The longitudinal proton speeds are (a) $v = 3$ a.u., (b) $v = 5$ a.u., and (c) $v = 8$ a.u., while the proton yield at ZDF is obtained by collecting all transverse proton speeds such that $v_t < 10^{-5}$ a.u.

yield when the nanotube is in SiO_2 . This is consistent with the fact that, in Fig. 9(b), we are very close to the first ZDF peak in vacuum for this proton speed and nanotube length. On the other hand, in the case $v = 5$ a.u. and $L = 0.5 \mu\text{m}$, shown in Fig. 5(b), and in the case $v = 8$ a.u. and $L = 0.8 \mu\text{m}$, shown in Fig. 6(b), we notice that the yields of the central maxima when the nanotubes are in SiO_2 are about three times the yields for the nanotubes in vacuum. This can now be explained by noticing that, for these combinations of proton speed and nanotube length, the yields are very close to the first ZDF peaks in, respectively, Figs. 9 (b) and (c) for nanotubes in SiO_2 .

The results presented so far may be further elucidated by considering the effects of the surrounding medium on typical proton trajectories in carbon nanotubes, as displayed in Figs. 10 and 11. We note that, in the case without image potential, there is only one type of proton trajectory, arising from proton oscillations between the opposite sides of the nanotube wall. In this case, the angular distributions of channeled protons through different (11, 9) nanotubes are similar for the same dwell times L/v , and their widths obey the law $v \cdot \Theta_w = \text{constant}$ for different protons speeds. When the image potential is included, there are two characteristic types of proton trajectories, arising from proton oscillations between the opposite sides of the nanotube wall, and proton oscillations in the potential minima generated by the image potential.

Figure 10 shows dependence of the proton deflection angle Θ_x multiplied by the proton speed v on the dwell time L/v for an impact parameter of $x_0 = 12$ a.u. and three different proton speeds (a) $v = 3$ a.u., (b) $v = 5$ a.u. and (c) $v = 8$ a.u. for a nanotube in vacuum and encapsulated by SiO_2 . Since protons with impact parameters $|x_0| \geq 11$ a.u. have enough transversal energy to make oscillations between the opposite sides of the nanotube wall, the results shown in Fig. 10 resemble the motion of a particle in a box with rigid walls owing to our use of the Doyle-Turner potential. The amplitude of the oscillations incrisies slightly due to weakening of the image forces with increasing proton speed. More importantly, we see very little influence of the dielectric surrounding on the type of trajectories shown in Fig. 10, even at higher proton speeds or after multiple oscillations of inside the nanotube.

Figure 11 shows the dependence of the proton deflection angle Θ_x multiplied by the proton speed v on the dwell time L/v for two proton impact parameters, $x_0 = 3$ a.u. and $x_0 = 8$ a.u., and three protons speed (a) $v = 3$ a.u., (b) $v = 5$ a.u. and (c) $v = 8$ a.u., for a nanotube in vacuum and encapsulated by SiO_2 . Protons with impact parameters $|x_0| \leq 11$ a.u. do not have enough transversal energy to bounce between the opposite sides of the nanotube wall, but rather undergo oscillations in the transverse plane around the minima generated by the image potential near $x \approx 9.3$ a.u. It is obvious from Figure 11 that the amplitudes of these oscillations decrease

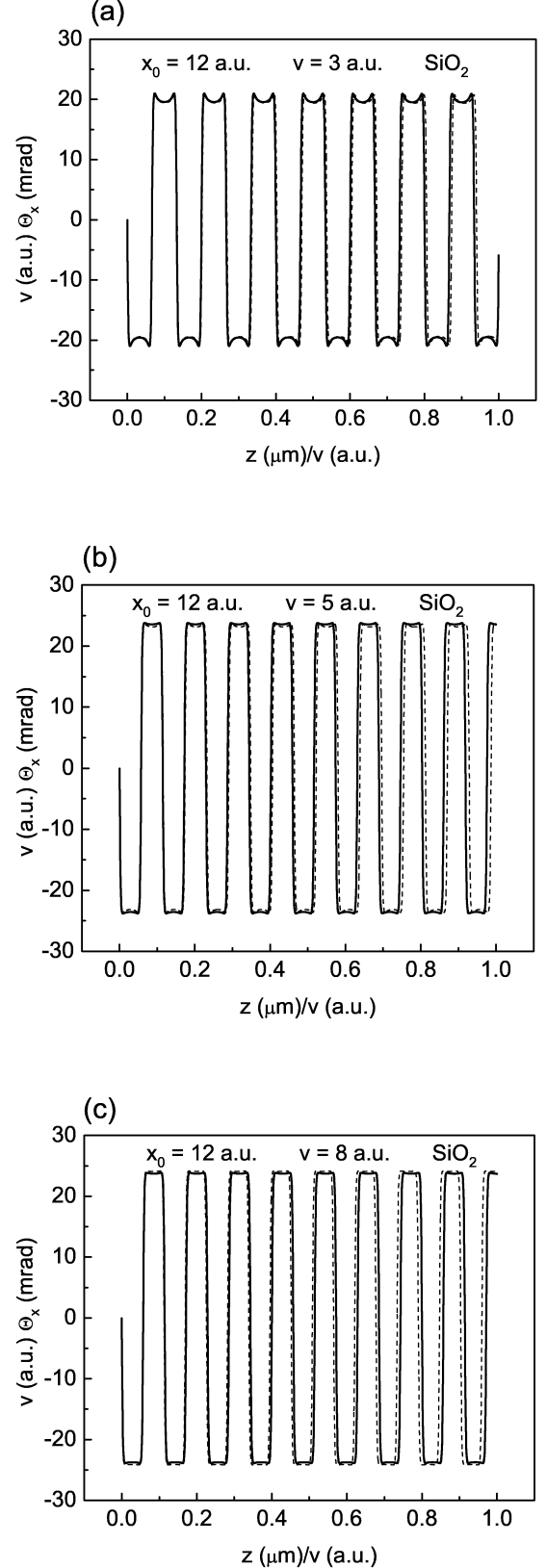


FIG. 10: Dependence of the proton deflection angle Θ_x in mrad multiplied by the proton speed v in a.u. on the dwell time L/v (in units of $\mu\text{m}/v_b = 0.4571$ ps) for a proton impact parameter of $x_0 = 12$ a.u. and the three protons speeds (a) $v = 3$ a.u., (b) $v = 5$ a.u. and (c) $v = 8$ a.u., due to an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by SiO_2 channels (solid curve).

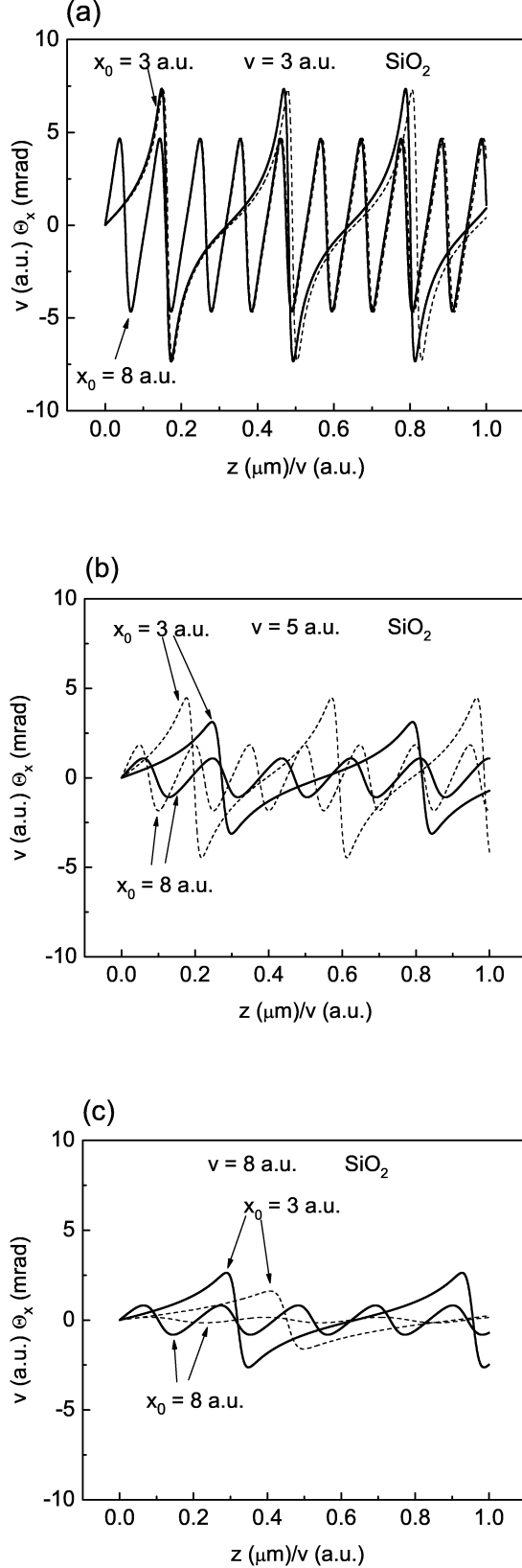


FIG. 11: Dependence of the proton deflection angle Θ_x in mrad multiplied by the proton speed v in a.u. on the dwell time L/v (in units of $\mu\text{m}/v_b = 0.4571$ ps) for proton impact parameters of $x_0 = 3$ a.u. and $x_0 = 8$ a.u. and three proton speeds (a) $v = 3$ a.u., (b) $v = 5$ a.u. and (c) $v = 8$ a.u., due to an (11, 9) SWNT in vacuum (dashed curve) and encapsulated by SiO_2 channels (solid curve).

and their periods increase with increasing proton speed, which is easily explained by the weakening of image force as shown in Figures 1 and 2. On the other hand, such changes in the image interaction did not give any substantial effects in Figure 10 because the total potential is dominated by the repulsive interaction for proton's impact parameters $|x_0| \geq 11$ a.u., as is obvious from Figure 2. However, more important properties seen in Figure 11 are the strong effects of dielectric media on oscillations in the proton deflection angle at the speeds $v = 5$ a.u. and $v = 8$ a.u. Namely, one notices in Figures 11 (b) and (c) that the shapes of oscillations for nanotubes in SiO_2 do not change much between those two speeds, whereas the periods of oscillations for nanotubes in vacuum have much shorter periods for $v = 5$ a.u., and much longer periods for $v = 8$ a.u. than those in the SiO_2 cases. These notions can be related to the appearance of ZDF peaks in Figures 9 (b) and (c), as well as to the values of forces shown in Figures 2 (b) and (c) for the same systems.

IV. CONCLUDING REMARKS

We have presented the first theoretical investigation of the effects of dynamic polarization of the carbon atom's valence electrons on the angular distributions of protons channeled in an (11, 9) SWNT surrounded by different dielectric media. Proton speeds between 3 and 10 a.u., corresponding to energies of 0.223 and 2.49 MeV, have been chosen, with the nanotube's length varied between 0.1 and 1 μm .

We have confirmed here our earlier findings that in short chiral SWNTs, it is the dynamic image interaction that gives rise to the rainbow effect in the angular distributions of protons channeled at the speeds below some $v \approx 8$ a.u. [6]. In the presence of dielectric media, this range of the image interaction effects is expanded to higher proton speeds because then the SWNTs become "transparent" to the polarization effects of the surrounding material. On the other hand, for proton speeds below $v \approx 3$ a.u., the image interaction is almost unaffected by the surrounding media because of the efficient screening by the nanotube.

Specifically, we have found that the effects of dielectric media are not only of quantitative nature in affecting the positions of the rainbow peaks, but rather can give rise to qualitative differences compared to the case of nanotubes in vacuum, e.g., in yielding different numbers of rainbow peaks for the same proton speed and nanotube length. For example, we have seen that the presence of dielectric media in our simulations both removes (see Figure 3(b)), and introduces (see Figures 5-8(b)) rainbow singularities in the angular distributions of protons channeled through nanotubes. Moreover, the type of the surrounding material has also been found to affect details of the proton angular distributions.

Going further beyond our previous study [6], we have analyzed here the zero-degree focusing (ZDF) effect and

found quite substantial differences between the cases of nanotubes in vacuum and in dielectric media when it comes to the periods of peaks in the proton yield as a function of dwell time through the nanotube. These effects have been further analyzed by studying typical proton trajectories which revealed strong effects of dielectric media. Because it may be easy to measure such features of ZDF in future experiments on ion channeling through carbon nanotubes, we shall devote a separate study to the ZDF in chiral SWNTs as particularly simple prototypes of quasi-one-dimensional channeling where the image interaction produces rich structures in the angular distributions of channeled ions.

All our findings indicate that it is important to carefully consider in future simulations and experiments the role played by dielectric media in ion channeling through carbon nanotubes at the MeV energies. For example, the best well ordered carbon nanotubes have been grown in porous dielectric media, such as Al_2O_3 , so that in any analysis of ion channeling experiments through such structures one may not realistically ignore the influence of dielectric media. Moreover, in the experiment by Zhu *et al.* [2], angular distributions of ions channeled through the nanotubes grown inside the pores in Al_2O_3 were compared with those coming from ion channeling through the pores of pristine Al_2O_3 [2]. It is therefore important to perform comparative simulations of ion channeling through channels in different materials, with and without carbon nanotubes embedded in them, while taking proper account of the dynamic polarization effects. While a detailed study of this problem is in progress,

some qualitative predictions can be made here for channels inside conducting materials. Based on recent calculations of the dynamic polarization of such structures [30, 31, 32, 37], it follows that the image force would be expected to play similar role as described in the present work, at least judging by its magnitudes for a nanotube in vacuum and for an empty channel in metal having the same radius as nanotube (compare thin solid lines with dashed lines in Fig.1(c)). However, it is questionable whether the atomic structure of walls in such channels would be smooth enough to support the rainbow effect [19, 31, 32]. This leaves the ZDF as probably the most robust feature associated with the image force, which could be probed with comparable degrees of experimental detail for ion channeling through both pristine channels and carbon nanotubes grown in those channels. We finally note that such studies may further elucidate dielectric properties of carbon nanotubes in the presence of dielectric media of relevance to nanoelectronic, such as SiO_2 .

Acknowledgments

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